

A non-parametric and scale-independent method for cluster analysis II: the multivariate case

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ABSTRACT

A general method is described for detecting and analysing galaxy systems. The multivariate geometrical structure of the sample is studied by using an extension of the method which we introduced in a previous paper. The method is based on an estimate of the probability density underlying a data sample. The density is estimated by using an iterative and adaptive kernel estimator. The used kernels have spherical symmetry, however we describe a method in order to estimate the locally optimal shape of the kernels. We use the results of the geometrical structure analysis in order to study the effects that it has on the cluster parameter estimate. This suggests a possible way to distinguish between structure and substructure within a sample.

The method is tested by using simulated numerical models and applied to two galaxy samples taken from the literature. The results obtained for the Coma cluster suggest a core-halo structure formed by a large number of geometrically independent systems. A different conclusion is suggested by the results for the Cancer cluster indicating the presence of at least two independent structures both containing substructure.

The dynamical consequences of the results obtained from the geometrical analysis will be described in a later paper.

Further applications of the method are suggested and are currently in progress.

Subject headings: methods: numerical - galaxies: clustering - galaxies: structure.

1. Introduction

Cluster analysis includes a rather rich list of methods that mathematical statistics offers in order to group sample data into simpler subunits (e.g. Murtagh & Heck, 1987; Pisani, 1994, hereafter paper I, and references therein). Within the astronomical and astrophysical context, cluster analysis can be applied to galaxy samples spanning large scale volumes in order to detect systems generally termed groups and clusters of galaxies. On the other hand, by studying small-scale volumes containing rich concentrations of galaxies it is possible to analyse substructures within systems (i.e. clusters) of galaxies. As was described in paper I, the methods of cluster analysis can be broadly divided into two families: parametric and non-parametric methods. In astronomy, non-parametric methods are hardly ever used. On the other hand there is a very rich literature of examples of applications of parametric methods. These methods generally work in the following way. First it is necessary not only to define what a system is operationally, but also to give a critical or fiducial value of a particular parameter that can be estimated for each system such as, for example, the local luminosity density of galaxy groups as in Tully (1980, 1987) or the separation in velocity and angular coordinates as in Huchra & Geller (1982, and more recently Ramella, Geller & Huchra 1989). Then the parametric method detects only those systems whose parameter is larger than a given threshold. It is not difficult to understand that within this framework a lot of parameters can be taken and an arbitrary choice of the critical parameter can lead to an author-dependent catalogue of systems. This family of methods is well suited to detecting structures that are well known in advance, but they risk introducing strong biases if the features of the systems to be detected are not well known as is the case for galaxy clustering in astronomy. These facts are the main cause of the disagreement that exists among the results obtained by several authors in both large scale cluster analysis and small scale substructure analysis (see e.g. paper I).

In order to overcome these problems, we propose here a method that satisfies the following requirements: a) it is non-parametric, in the sense that no particular assumption needs to be made concerning the number, shape or any parameter or feature of the systems that are supposed to be detected; b) it gives an estimate of the statistical significance according to which the detected systems can be distinguished from noise fluctuation; c) it gives an estimate of the probability that a given galaxy is a member of a given system, for all galaxies and all systems; this information can be used to detect interlopers within systems; d) it can be used to infer considerations about the dynamics of the systems within the data sample, at least in the case that galaxy catalogues are being considered. Hence the structure of the method consists of a geometrical analysis whose results are the basis of the subsequent dynamical analysis. We must stress that the geometrical analysis of

the clustering structure of galaxy samples assumes that the velocity of a galaxy is a pure radial coordinate. This assumption is trivially false within a gravitationally bound system; however without assuming this the geometrical analysis cannot be done. We will discuss the effects of this assumption in the dynamical part of the analysis that will be presented in a future paper.

The main mathematical details of the univariate version of the method we propose are described in paper I. In the present paper we consider the multivariate extension of the method. The geometrical clustering analysis is based on the estimate of the probability density function underlying the data sample. The extension of this estimate can profitably be used to study cosmological density fields. This and other applications of the method are currently in progress.

The present paper is structured as follows. In §2 the extension of the univariate non-parametric method described in paper I to the general multivariate case is described. In §3 we consider the problem of estimating the density of a highly elongated system by using spherical kernels. In §4 a correction is presented and tested for taking into account the local optimal shape of kernels in the density estimate. We describe in §5 a modified version of the Kittler (1976) mapping. This mapping is basically a visualization tool, but it can be used profitably for obtaining information concerning the effects that the detected structure has on some relevant cluster parameters. In §6 we consider a possible way to distinguish between the presence of structure and substructure within a given sample. In §7 we describe the general structure of the method of clustering analysis we propose. In §8 and 9 we report the results obtained from the analysis of two well known galaxy clusters. In this paper we consider only galaxy samples spanning small scale volumes. The analysis of galaxy samples spanning large volumes will be treated in a future paper. Finally, §10 summarizes the main points and the results obtained.

2. The extension to the multivariate case

2.1. The estimate of the probability density and the definition of cluster

In principle, the extension of DEDICA (paper I) to the case of a number of dimensions d larger than one is trivial. In fact, the fundamental relations used in paper I hold in d dimensional spaces in the following form.

With reference to the definitions given in §3.1 of paper I, we suppose that we have a sample D_N of N points with position vectors $\vec{r}_i \in \mathbb{R}^d$, ($i = 1, \dots, N$). If σ_i is the kernel

width of the i^{th} point, the adaptive kernel density estimate $f_{ka}(\vec{r})$ is given by:

$$f_{ka}(\vec{r}) = \frac{1}{N} \sum_{i=1}^N K(\vec{r}_i, \sigma_i; \vec{r}) \quad (1)$$

where \vec{r} are position vectors and we consider the Gaussian kernel:

$$K(\vec{r}_i, \sigma_i; \vec{r}) = \frac{1}{(\sqrt{2\pi}\sigma_i)^d} \exp \left[-\frac{1}{2} \frac{|\vec{r}_i - \vec{r}|^2}{\sigma_i^2} \right]. \quad (2)$$

In order to completely specify the density estimate $f_{ka}(\vec{r})$ we have to describe the procedure for estimating the kernel widths σ_i . We adopt here the same procedure described in paper I: the local minimization of the integrated square error:

$$ISE[f] \equiv \int_{\mathfrak{R}} [F(\vec{r}) - f(\vec{r})]^2 d\vec{r} \quad (3)$$

where $F(\vec{r})$ is the "true" probability density field. The use of a kernel designed to minimize the integrated square error in order to study the modal points of a distribution was addressed in paper I where we have obtained encouraging results for the univariate case. It is easy to note that:

$$ISE[f] = \int_{\mathfrak{R}} F^2(\vec{r}) d\vec{r} + \int_{\mathfrak{R}} f^2(\vec{r}) d\vec{r} - 2 \int_{\mathfrak{R}} F(\vec{r}) f(\vec{r}) d\vec{r} \quad (4)$$

and hence the minimization of $ISE[f]$ is equivalent to the minimization of the cross validation $M(f)$ defined by:

$$M(f) \equiv \int_{\mathfrak{R}} f^2(\vec{r}) d\vec{r} - 2 \int_{\mathfrak{R}} F(\vec{r}) f(\vec{r}) d\vec{r}. \quad (5)$$

It is possible to show that, under mild assumptions, $M(f)$ can be expressed as a function of the sample data positions \vec{r}_i and kernel widths σ_i (see paper I and references therein).

The iterative method which we propose for selecting the kernel widths of eq.(1) is the following:

1. set the first guess of the size $\sigma_{n=0} = 4\sigma_t$, where σ_t is the rule-of-thumb prescription for σ , see eq. (6) (note that there is no particular reason to choose the factor four in the previous equation, the aim is to start with a large value of σ_0),
2. take the value at the n^{th} iteration to be $\sigma_n = \sigma_{n-1}/2$
3. take the adaptive kernel estimate $f_{ka}^{(n)}(\vec{r})$ defined by

- $f_p(\vec{r}) = \text{fixed kernel estimate with kernel sizes } \sigma_i = \sigma_n \forall i$
 - sensitivity $\alpha = 1/2$ (see paper I for further details)
4. compute the value of $M(f_{ka}^{(n)})$
 5. finally select the optimal σ_n by minimizing the value of $M(f_{ka}^{(n)})$ and take the corresponding $f_{ka}(\vec{r})$ as the optimal density estimate.

By examining the tests we have done, it turned out that less than ten steps ($n \leq 10$) are enough to reach the optimal size, in agreement with the behaviour of this procedure found for the univariate case examined in paper I.

The rule-of-thumb estimate of the kernel size σ_t is given by:

$$\sigma_t = A(K)N^{-\frac{1}{d+4}}\sqrt{\frac{1}{d}\sum_{l=1}^d s_{ll}^2} \quad (6)$$

where s_{ll} is the standard deviation of the l^{th} coordinate ($l = 1, \dots, d$) of the sample data. The constant $A(K)$ depends only on the kernel and for the Gaussian case can be taken as 0.96 (Silverman 1986).

To complete the extension of the density estimate to the multivariate case it is sufficient to give the expression for the cross validation:

$$M(f) = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N K^{(2)}(|\vec{r}_i - \vec{r}_j|; \sigma_i, \sigma_j) - \frac{2}{N(N-1)} \sum_{i=1}^N \sum_{j \neq i} \frac{1}{\sigma_j^d} k\left(\frac{|\vec{r}_i - \vec{r}_j|}{\sigma_j}\right) \quad (7)$$

where

$$k(t) = \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2}t^2\right) \quad (8)$$

and

$$K^{(2)}(t; \sigma_i, \sigma_j) = \frac{1}{[2\pi(\sigma_i^2 + \sigma_j^2)]^{d/2}} \exp\left(-\frac{1}{2}\frac{t^2}{\sigma_i^2 + \sigma_j^2}\right). \quad (9)$$

We must stress that we adopt here the Gaussian kernel (eq. [2] and [8]) because it is differentiable in all its domain and this is a crucial feature in order to correctly use eq.(10) in order to find local maxima in the estimated probability density field eq. (1). However the Gaussian kernel is not the most efficient choice in order to minimize the $ISE[f]$. In fact the Epanechnikov kernel (Epanechnikov 1969) performs better, however Silverman (1986) shows that the values of the $ISE[f]$ obtained for these kernels are very similar. The choice of the radial dependence (exponential as for the Gaussian kernel or quadratic as for the Epanechnikov kernel) of the kernel $k(t)$ is not crucial in this sense, as far as $k(t)$ satisfies the

normalization and convergence conditions described in §3.1 of paper I (see also Silverman 1986). What is crucial for the $ISE[f]$ is the width of the kernels.

Finally we assume, as in paper I, that a peak in the density function indicates the presence of a cluster in the data. The position vectors of the peaks of the probability density estimate are defined as in paper I by the solution of the iterative equation:

$$\vec{r}_{m+1} = \vec{r}_m + a_d \frac{\vec{\nabla} f(\vec{r}_m)}{f(\vec{r}_m)} \quad (10)$$

with

$$a_d = \frac{d}{\sum_{i=1}^N \left[\frac{\vec{\nabla} f(\vec{r}_i)}{f(\vec{r}_i)} \right]^2} \quad (11)$$

(see Fukunaga & Hoestetler, 1975).

Since the limit $\vec{\varrho}$ of the sequence in eq. (10) generally depends on the initial value of the position vector $\vec{r}_{m=1}$:

$$\lim_{m \rightarrow +\infty} \vec{r}_m = \vec{\varrho}(\vec{r}_{m=1}) \quad (12)$$

we can label each point in the sample D_N by the limit $\vec{\varrho}_i = \vec{\varrho}(\vec{r}_{m=1} = \vec{r}_i)$ reached by the sequence in eq. (10) starting from the position of the i^{th} point. Then we can define the cluster C_μ as the set of all the points of D_N having the same label \vec{r}_μ and containing $n_\mu > 1$ points:

$$C_\mu = \{\vec{r}_i : \vec{\varrho}_i = \vec{\varrho}_\mu; n_\mu > 1\} \quad (13)$$

with $i = 1, \dots, N$ and $\mu = 1, \dots, \nu$ assuming that ν is the number of systems present within D_N .

The set of labels ϱ that are associated with only single points form the population of isolated points C_0 , hence:

$$C_0 = D_N - \bigcup_{\mu=1}^{\nu} C_\mu. \quad (14)$$

Equations (1) to (10) completely define the extension of the density estimation to the multivariate case. The scale independence of the present density estimate can be proved following the same argument used in paper I. The ability of the density estimate to describe highly elongated systems by using a centrally symmetric kernel is tested in §3 and 4.

2.2. The quantitative description of the clustering pattern

The statistical significance of the μ^{th} cluster \mathcal{S}_μ ($\mu = 1, \dots, \nu$) is defined as in paper I. In particular it is based on the assumption that the presence of the μ^{th} cluster produces a higher value of the local density and hence of the sample likelihood $L_N = \prod_i [\sum_{\mu=0}^\nu F_\mu(\vec{r}_i)]$ relative to the value L_μ :

$$L(\mu) = \prod_i \left[f_{ka}(\vec{r}_i) - F_\mu(\vec{r}_i) + \frac{1}{N} \sum_{j \in C_\mu} K(\vec{r}_j, \sigma_0; \vec{r}_i) \right] \quad (15)$$

that one would have if the members of the μ^{th} cluster were all isolated and hence belonging to the background component. A large value of the ratio L_N/L_μ characterizes the most prominent clusters. By using the likelihood ratio test it is possible to estimate the cluster significance \mathcal{S}_μ (Materne 1979 and references therein). The contribution to the local density $f_{ka}(\vec{r})$ due to the μ^{th} cluster is:

$$F_\mu(\vec{r}) = \frac{1}{N} \sum_{j \in C_\mu} K(\vec{r}_j, \sigma_j; \vec{r}) \quad (16)$$

(see also paper I), and the kernel size of the background component is estimated by:

$$\sigma_0 = \max_i \{\sigma_i\} \quad (17)$$

which is only slightly different from the estimate given in paper I, where σ_0 was defined as the average width of the kernels associated to the isolated data points. The set of the n_μ members of the μ^{th} cluster is indicated by C_μ . The function $F_\mu(\vec{r})$ is defined as in paper I.

Another modification compared to paper I concerns the estimate of the membership probabilities $P(i \in \mu)$ that the i^{th} point is member of the μ^{th} cluster. As the dimensionality d of the sample data increases, the discreteness effect due to the fact that we observe points and not a continuous function causes the i^{th} kernel $K(\vec{r}_i, \sigma_i; \vec{r}_i)$ to give a larger and larger contribution to $f_{ka}(\vec{r}_i)$ as d grows. This fact however does not necessarily mean that the "real" probability of isolation of the i^{th} point is larger for larger d . A general multivariate estimate of $P(i \in \mu)$ can be obtained by noting that the isolated points have:

$$f_{ka}(\vec{r}_i) \sim \frac{1}{N} K(\vec{r}_i, \sigma_0; \vec{r}_i). \quad (18)$$

In eq. (15) we estimate that the background density field is given by:

$$F_0(\vec{r}) = \frac{1}{N} K(\vec{r}, \sigma_0; \vec{r}). \quad (19)$$

which supports eqs. (15) and (17).

This suggests to define the probability that a given point is isolated, and hence due to the background component, as:

$$P(i \in 0) = \frac{\frac{1}{N}K(\vec{r}_i, \sigma_0; \vec{r}_i)}{f_{ka}(\vec{r}_i)}. \quad (20)$$

Numerical tests have shown that this expression is a more general estimate of the isolation probability than the definition adopted in paper I. However the two definitions are quite similar for $d = 1$. The difference between the definition adopted here and the one given in paper I is due to their different choice of the σ_0 value.

The probability that the i^{th} point is not isolated can be estimated as:

$$P_i = P(i \notin 0) = 1 - P(i \in 0) = \sum_{\mu=1}^{\nu} P(i \in \mu), \quad (21)$$

in order to satisfy the normalization constraint: $\sum_{\mu=0}^{\nu} P(i \in \mu) = 1$ (see Matérne, 1979). This definition is also in agreement with the prescriptions of the Neyman-Pearson theory of tests (see e.g. Ledermann 1984, vol. VI, pag. 278).

Moreover we assume that:

$$P(i \in \mu) \propto F_{\mu}(\vec{r}_i). \quad (22)$$

We adopt the following definition:

$$P(i \in \mu) = P_i \frac{F_{\mu}(\vec{r}_i)}{f_{ka}(\vec{r}_i)} \quad (23)$$

in other words the probability that a point is a member of a structure is distributed among the clusters according to the contribution to the total density due to each cluster.

The given definitions of $P(i \in 0)$ (eq.[20]) and $P(i \in \mu)$ (eq.[23]) are an extension to the kernel density estimate of the similar quantities defined in the general case by Matérne (1979). Our definitions inherit the features of asymptotical optimality of the kernel density estimator and hence are well suited as a non-parametric test to efficiently recognize and eventually remove background fluctuations as numerical tests have indicated. The efficiency of $P(i \in 0)$ and P_i estimates in order to detect the background component shown in the example discussed in §4. Recently Ramella et al. (1995) have used our prescription for $P(i \in 0)$ and $P(i \in \mu)$ in order to identify outliers in groups of galaxies. They have also applied other statistical methods and dynamical simulations. Their results support our prescription.

2.3. A measure of the overlapping among clusters

It is often useful to have a measure of how close the clusters are to each other. We want here to propose an estimate of the overlapping measure for the multivariate case that is non-parametric and not only pairwise. To this aim we introduce the following definitions. Suppose that we consider the μ^{th} cluster C_μ containing n_μ members. For each member $i_\mu \in C_\mu$ we can estimate $P(i_\mu \in 0)$ and $P(i_\mu \in \lambda)$, with $\lambda = 1, \dots, \nu$. The interlopers (or outliers) are defined as the members that satisfy the following relation:

$$P(i_\mu \in 0) \geq P(i_\mu \in \mu) \quad (24)$$

in other words they are more probably isolated points than cluster members.

In the case that for at least one cluster $\lambda \neq \mu$ we have

$$P(i_\mu \in \lambda) \geq P(i_\mu \in 0) \quad (25)$$

for some $i_\mu \in C_\mu$, then there are some members of the μ^{th} cluster that could have been classified as members of the λ^{th} cluster. In other words for some members of the μ^{th} cluster the probability P_{i_μ} to be part of a structure is not entirely due to the presence of only one cluster. In this case we can say that the μ^{th} and the λ^{th} cluster are in contact: they somehow share some members, they are not completely disjoint. We express this relation by the notation:

$$\mu \rightarrow \lambda. \quad (26)$$

It is easy to see that the μ^{th} cluster can be in contact with several clusters. The strength $\mathcal{L}(\mu, \lambda)$ of the contact can be measured by

$$\mathcal{L}(\mu, \lambda) = \sum_{i_\mu \in C_\mu} P(i_\mu \in \lambda) + \sum_{i_\lambda \in C_\lambda} P(i_\lambda \in \mu). \quad (27)$$

We can also see that the contact may be a non-symmetric property of clusters. In other words, if the μ^{th} cluster is in contact with the λ^{th} cluster it is not necessarily true that the λ^{th} cluster is in contact with the μ^{th} cluster. This is formally due to the fact that eq.(25) is not symmetric in λ and μ . Asymmetric contact may occur between a significant and compact cluster and a non significant loose cluster that happens to fall close enough to the first cluster.

In the case of symmetric contact we write:

$$\lambda \leftrightarrow \mu. \quad (28)$$

The above definitions are crucial for examining substructured and elongated clusters.

3. The effect of anisotropy

As introduced in the previous section, we want to examine here the following question: how reliable is the estimate of the density of an elongated system obtained by using centrally symmetric kernels?

The analytical answer to this question comes from a theorem (Fukunaga 1972, Silverman 1986) that proves the following statement. Suppose we have a multidimensional and unimodal system with covariance matrix \mathcal{A} . If we adopt a kernel estimate of the probability density, then the $ISE[f]$ is reduced if we change the metric of our space. Instead of the usual euclidean metric, represented by the unit matrix \mathcal{I} , it is more convenient to use the metric represented by the inverse of the covariance matrix \mathcal{A}^{-1} . This result holds independently of the kind of kernel adopted (not necessarily Gaussian, Silverman 1986). If \mathcal{A} is not the identity matrix \mathcal{I} , we can change the metric of our space by: $\vec{y} = \mathcal{W}\vec{r}$. Here \mathcal{W} is the $d \times d$ matrix that describes the transformation taking the covariance matrix of the data into the identity matrix. This transformation is also called whitening (Fukunaga 1972). The statement of the theorem is equivalent to saying that in the whitened space the centrally symmetric kernel (see eq. [8]) has the optimal¹ shape, in the sense that it gives a smaller value of the $ISE[f]$ relative to the original metric (or shape). The expression for the kernel density estimate taking into account the change in the metric is indicated in the next section (eq. [30]).

By using $N_s = 1000$ Monte Carlo simulations of a model density field $F(x, y)$ with $N_p = 500$ points we have tested the performance of the density estimator described on §2 for systems with rather different anisotropies. The goodness of the density estimate is measured by:

$$\Delta = \frac{1}{100 \times 100} \sum_{i=1}^{100} \sum_{j=1}^{100} [F(x_i, y_j) - f_{ka}(x_i, y_j)]^2 \quad (29)$$

for each simulation. In our tests we have taken for the model field $F(x, y)$ a bivariate Gaussian with several values of the axial ratio a/b . The relevant statistical parameters of Δ are reported in table 1 for several values of a/b . In each simulation the model field has unit variance along the major axis, while the kernels are centrally symmetric. The results of the simulations are shown in Figs. 1 and 2 (mean values are plotted). In Fig. 1 we show the results obtained in the case of a centrally symmetric model density field $F(x, y)$ and by using a Gaussian kernel with the same central symmetry. In Fig. 2 we show the case

¹In general, the optimality of the kernel estimate is referred to asymptotic conditions, i.e. in the limit $N \rightarrow +\infty$ (see paper I and references therein).

of a model density field with an elliptical shape with axis ratio $a/b = 0.1$, while the used kernels are Gaussian with central symmetry and hence do not have the same shape of the model field (they are not optimal). It appears that in the case where the kernel has the locally optimal shape (Fig. 1) the estimate is rather accurate, confirming the quoted theorem. In the case of a kernel which does not have the optimal shape (Fig. 2) rather rounder isoplethes are obtained. However the estimate of the density is still good. The quantity that is more sensitive to the non-optimality of the kernel shape is the gradient of the density. In the next section we show that it can fluctuate quite widely as will be illustrated in the example given. We do not report the results of the test in the case that both the data and the kernels have the same value of axis ratio $a/b < 1$ since in that case the whitening procedure make this test equivalent to what obtained in the case $a/b = 1$. We note that the value of N_p used in our simulations is rather high relative to the size of usual observational samples (see § 8 and 9). The aim of these simulations is to illustrate the two different behaviours of the kernel density estimator when the kernel shape is optimal and when it is not, in the asymptotic limit. We also note that for asymptotic conditions we assume we have no problems in the estimate of the covariance matrix, contrary to what is likely in real situations. In the next section we analyse the problems that arise when dealing with smaller anisotropic systems imbedded in an isotropic background.

4. An estimate of the locally optimal metric

The message contained in the theorem of the previous section is that in the general multimodal case, each sample point should be associated with a matrix which defines the locally optimal (in the sense discussed in § 2.1 and § 3, for further details see Fukunaga, 1972) metric, estimated from the covariance matrix of the system to which the point belongs. Unfortunately we do not know this information in advance. In order to save the non-parametric nature of the present method, we should avoid all a priori guesses concerning the number of systems present in our sample and the membership of each point.

We propose a way out of this problem based on very simple remarks. Let us consider the following example in order to clarify the whole procedure. We consider for the moment only $d = 2$ samples because of their easy geometrical visualization. In Fig. 3 a $d = 2$ sample is shown. It contains 100 points obtained by a Monte Carlo simulation of an unimodal system with a bivariate Gaussian profile, axis ratio $a/b = 0.1$ and position angle $\theta = 45^\circ$. Superimposed on this system there is a population of 100 points randomly distributed. A straightforward application of the $d = 2$ version of DEDICA described in § 2 indicates the presence of $\nu = 26$ clusters and $n_0 = 0$ isolated points (see Fig. 4). The density estimate $f_{ka}(x, y)$ is shown in Fig. 5. In table 2 we report the richness and significance of each

cluster. Our experience and a conservative point of view suggests we consider a cluster as real if its significance is larger than 0.995 in the case of a sample without isolated points, while a cutoff of 0.99 may be adopted for samples containing isolated points. This is caused by the fact that in a sample without isolated points the value of σ_0 (eq. [17]) may be underestimated. As a general empiric rule (see Materne 1979; Ledermann 1984 vol. VI pag. 278-282) the value 0.99 can be assumed.

From an inspection of Fig. 4 and 5 it appears clear that the disagreement between the central symmetry of the kernel used and the locally optimal metric has caused the elliptical system to be artificially fragmented into several subsystems aligned along the major axis of the simulated model profile. We can also notice that the spurious subsystems are quite close to one another and it is easy to guess that the density estimates of these subsystems should show a certain mutual contact (see also Fig. 6). By merging the systems that are in mutual contact we may be able to recover the true elongated system and hence the locally optimal metric. Spurious contacts due to non-significant clusters and/or isolated points must be avoided in order to prevent biases in the estimate of the covariance matrix.

We adopt the following procedure:

1. take the first estimate of the clustering structure of the sample by using centrally symmetric kernels, hence obtaining a catalogue of clusters and isolated points,
2. remove from the catalogue all the non-significant clusters and isolated points,
3. check if the remaining systems are in contact and merge all the clusters that show mutual contact, thus obtaining a new catalogue of clusters,
4. consider the new clusters resulting from merger of previous distinct clusters, check if these clusters are unimodal by applying DEDICA to the whitened coordinates of the cluster members. If the new cluster is unimodal, estimate the covariance matrix of the cluster and hence the locally optimal metric. Otherwise, keep the previous local metric,
5. consider the new estimate of the density by taking into account the new local metric determined in the previous step and check if the new density estimate causes different clusters to be in contact; if so, return to previous step,
6. if no further merging occurs, then the locally optimal metric of each point can be estimated from the covariance matrices of the merged clusters $\mathcal{A}_i \neq \mathcal{I}$, while for the non-merged and non-significant clusters \mathcal{A}_i is assumed to be the identity \mathcal{I} . The final

density estimate is:

$$f_{kaw}(\vec{r}) = \frac{1}{N} \sum_i \frac{(\det\{\mathcal{A}_i\})^{-1/2}}{(\sqrt{2\pi}\sigma_i)^d} \exp \left[-\frac{1}{2} \frac{(\vec{r} - \vec{r}_i)^T \mathcal{A}_i^{-1} (\vec{r} - \vec{r}_i)}{\sigma_i^2} \right]. \quad (30)$$

where w signifies whitened.

We can obtain the final classification by using the peak determination equation (10) applied to $f_{kaw}(\vec{r})$.

In general we have found that this procedure converges quite rapidly (only one iteration !) to the locally optimal metric. Let us now see how it works in the trial sample described above. By inspection of table 2, it can be seen that the clusters 1, 2, 8, 9, 12, 14 and 17 have significance larger than 0.995 while the cluster number 19 has a significance of 0.991. If we include the cluster 19 in the set of significant clusters, adopting the weak limit of the significance, we obtain the results reported in table 3 after the contact test: all the clusters are in mutual contact, hence they are probably part of only one system that may be elongated and/or substructured. By performing the test of modality, we can see that the merged cluster obtained at the step 4 of the above procedure is not unimodal. Hence the list of clusters that we have merged is either a collection of actually different clusters close to one another, or we have included in the list of significant clusters some spurious systems that have biased the estimate of the locally optimal metric. To clarify this point we examine the result of the contact test reported in table 3. It can be seen that cluster 19 shows a quite different behaviour from all the others. It has only asymmetric contacts with other clusters and it shows contact strength nearly an order of magnitude weaker than for the other clusters. Finally it has the smallest value of the significance S_μ and it is characterized by a low value of $P(i \notin 0)$. The contours plotted in Fig. 7 also show that the cluster $\mu = 19$ should be considered as detached from the other significant clusters. These remarks suggest that we re-perform the merging after having removed the cluster $\mu = 19$. In this case we find that all of the clusters considered merge to form a unique unimodal structure. The estimate of the local metric is a rather good approximation of the simulated model. In Fig. 8 we show the plot of the density $f_{kaw}(x, y)$ taking into account the locally optimal metric. Eventually we can apply the peak identification algorithm (eq. [10]) to check if the membership of the non-merged part of the catalogue, discarded in step 2, changes or not. In general this could produce only minor changes in the membership assignments.

We have preferred to apply the above method, that will whiten the data sample only in the case of a positive outcome of the contact test, instead of an unconditioned whitening of the data sample because it analyses more carefully the data structure. We have applied the quoted procedure to several multimodal $d = 2$ samples and also to rich and poor $d = 3$

samples always obtaining good results. Hence the reliability of the procedure which we are proposing is well confirmed.

5. The Kittler mapping

Here, we introduce a useful tool for representing the structure of multivariate data sets. We can roughly say that the aim of this tool is to construct a path through the data set that takes as many as possible data points near a particular mode (peak), in the estimated probability density \hat{f} , before moving to another nearby mode. At each step in the sequence the next point is selected within "nearby" data points so that one moves as far uphill or as little downhill on \hat{f} as possible. This procedure gives a path that follows the highest gradient of \hat{f} when approaching a mode, while it follows the smallest gradient when it goes away from a mode (see e.g. Silverman 1986). The original method is due to Kittler (1976), while we are using a slightly modified version. We refer to the original Kittler (1976) paper for the full set of theorems underlying this mapping. In this section we only show the new version of the Kittler mapping we have introduced. In fact the aim of the method was to identify peaks in a general multivariate probability density field estimated by the fixed kernel method (Parzen, 1962). As a consequence, the Kittler method inherits the problems of the fixed kernels estimator of the probability density (see discussion in paper I and references therein). At variance with the original Kittler paper, we adopt the density estimate f_{ka} described in § 2 and the peak identification procedure described in paper I and its extension to the general multivariate case outlined in § 2. We are using the Kittler mapping as a useful tool for visualizing the structure of a multivariate data set and to order a generally multimodal set of points by non-increasing density within connected overdense regions.

In practice, the Kittler mapping (hereafter KM) is a particular rearrangement $k = KM(i)$ of the data sample $D_N = \{\vec{r}_i : i = 1, \dots, N\}$:

$$KM : D_N \rightarrow \mathcal{K} \quad (31)$$

Let us suppose that the probability density field associated with this set is estimated by eq. (1). According to Kittler, it is possible to choose arbitrarily the first point of the sequence $\mathcal{K} = \{\vec{r}_k : k = KM(i), i = 1, \dots, N\}$, however we prefer to start with the highest probability point:

$$\vec{r}_{k=1} = \vec{r}_{i_{max}} \quad (32)$$

or $1 = KM(i_{max})$, where i_{max} is defined by:

$$f_{ka}(\vec{r}_{i_{max}}) \geq f_{ka}(\vec{r}_i), \quad \forall i \in [1, N]. \quad (33)$$

Then we can consider the set of points that are neighbours of $\vec{r}_{k=1}$. Among these points we can choose the next point $\vec{r}_{k=2}$ of the sequence \mathcal{K} as the one having the highest value of the density $f_{ka}(\vec{r})$, excluding the point corresponding to $\vec{r}_{k=1}$. At the next step, all of the points which are neighbours of the last point $\vec{r}_{k=2}$ of the sequence are also included as the set of neighbours among which the search of the highest density point is made. The procedure is repeated in this way for the other members of the set until no further neighbour is found. Since this may happen before all the data in the starting set has found a place in the sequence \mathcal{K} , we have introduced the convention that when the procedure breaks, it restarts with the point not yet present within the sequence that is the closest to the starting point $\vec{r}_{k=1}$. In order to completely define the procedure, we define two points \vec{r}_i and \vec{r}_j to be neighbours if the distance between them is not larger than the sum of the sizes of their corresponding kernels $h_i + h_j$ appearing in eq. (1):

$$|\vec{r}_i - \vec{r}_j| \leq h_i + h_j \quad (34)$$

similarly to the definition given by Kittler (1976). In order to keep the above relation as simple as possible, we have considered the Kittler mapping only by using the spherical kernel estimate of the density described by eq. (1). It is possible to extend the KM to non-isotropic kernels (eq. [30]), at the cost of longer computing time.

By considering the peak to which $\vec{r}_{k=1}$ belongs, the above mapping gives the sequence of points that would be obtained by cutting the $f_{ka}(\vec{r})$ hypersurface by hyperplanes of constant density at lower and lower values. When another nearby peak is reached the sequence of points reaches the highest density point following the steepest path and then re-descends through the remaining points as for the previous peak.

Once the sequence \mathcal{K} is obtained, it is possible to consider the plot: $\{(k, f_{ka}(\vec{r}_k)), k = KM(i), i = 1, \dots, N\}$ that shows in two dimensions the structure in the multivariate data set, as outlined in full mathematical detail by Kittler (1976). Although this procedure may be not rewarding in two dimensions (see Figs. 6 and 13) and is certainly not in one dimension, in our opinion it is very useful for visually examining data in three and higher dimensional spaces. However it is worth stressing that the modality of the density field $f_{ka}(\vec{r})$ and in the Kittler graph may not be exactly the same. This disagreement may occur for some peak that has a member falling in the low probability tail and, in that case, its distance from the nearest member of that peak may exceed the critical value defined in eq. (34). Because of this, we prefer to consider the DEDICA method (§2) in order to define the systems present within the data set.

6. Effects of structure and substructure

In this section we want to consider the effect that the presence of structure has on the estimate of a given parameter.

Let us consider the following example. Suppose we have a set S_1 (see Fig. 9) of N points in a the (x, y) space obtained by a random sampling of, say, a centrally symmetric and bivariate Gaussian with unit variance centered on $(3, 3)$ and let $f_{1,ka}(x, y)$ be the density estimated according to the method described in § 2.1. We arrange the data set in a sequence \mathcal{K}_1 in order of non-increasing density:

$$f_{1,ka}(x_k, y_k) \geq f_{1,ka}(x_{k+1}, y_{k+1}) \quad (35)$$

for $k = 1, \dots, N - 1$. Let us call $\sigma_{k,1}$ the value of the coordinate dispersion estimated from the first k points along the sequence \mathcal{K}_1 . This is equivalent to saying that $\sigma_{k,1}$ is the dispersion of the coordinates of the subset of points occupying the region defined by:

$$f_{1,ka}(x, y) \geq \delta_k \quad (36)$$

where $\delta_k = f_{1,ka}(x_k, y_k)$. In Fig. 10a we show the plot of $\sigma_{k,1}$ as a function of k for S_1 . The application of DEDICA shows the presence of one structure without isolated points. It can be seen that $\sigma_{k,1}$ grows quite smoothly with k . The fluctuations are mainly due to noise in the density and σ estimates. Let us consider now a second sample S_2 (see Fig. 9) containing $N = 100$ points obtained by a random sampling of a centrally symmetric and bivariate Gaussian with unit variance centered on $(0, 0)$. Let $f_{2,ka}(x, y)$ be the density estimate obtained for the sample S_2 . In this case DEDICA indicates the presence of two significant peaks (relative to a flat background) and no isolated points. However the two peaks are rather close to one another and their overlap is large. Both peaks have 50 members while there are 92 members shared by the two peaks with a value of the parameter $\mathcal{L} = 11.5$. It is worth stressing the fact that the presence of two different peaks is not due to a non-optimal shape of the kernels; in fact the kernels are centrally symmetric so their shape is optimal in the sense of the Fukunaga (1972) theorem (see §3). In this case the detected structure is due to random fluctuations in $f_{2,ka}(x, y)$. If we sort the S_2 points in the same way as for S_1 (eq.[35]), we obtain the sequence \mathcal{K}_2 . The value of the coordinate dispersion $\sigma_{k,2}$ along the \mathcal{K}_2 sequence grows quite smoothly with k . Moreover it can be seen in Figs. 10a and 11a that $\sigma_{k,1}$ and $\sigma_{k,2}$ both follow a rather smooth dependence on k although $\sigma_{k,2}$ is larger than $\sigma_{k,1}$. The jack-knife estimates of the uncertainties² $\Sigma(\sigma_{k,1})$ and $\Sigma(\sigma_{k,2})$ are similar (see Fig. 10b and 11b).

²Hereafter $\Sigma(p)$ indicates the jack-knife estimate (Efron & Tibshirani 1986) of the dispersion of the quantity p .

Finally, let us consider the sample $S = S_1 \cup S_2$ (see Fig. 9). If we arrange the data in order of non-increasing density as in the previous example, the points of the sequence jump continuously from one system to the other (see Fig. 12a). In order to avoid this problem and to sort points by decreasing density without mixing points that belong to overdense regions that are disconnected, we consider the following arrangement (the Kittler sequence): the first $k = 1$ point of the sequence \mathcal{K} is the one having the highest value of the density estimate, then from the k^{th} point the sequence moves along the $z = f_{ka}(x, y)$ surface³ to the next point not yet listed in the sequence following the shallowest path when descending from a density peak, while it follows the steepest path when rising to a peak. In Fig. 12b we show the sequence of the abscissae of the sample points along the Kittler sequence. It can be seen that the sequence first spans the overdense region defining the first peak then moves quickly to the top of the second peak and spans the remaining region of the second peak; finally it covers the underdense region surrounding both peaks (see also Fig. 13).

In Fig. 14a we show the plot of σ_k versus k along \mathcal{K} . It can be seen that σ_k grows smoothly until $k = 60$ where the sequence begins to include points belonging to the second peak. Then the value of σ_k and its dispersion $\Sigma(\sigma_k)$ (Fig. 14b) rise quickly. The value of σ_k finally saturates after the overdense region of the second peak is covered.

In conclusion it is possible to say that the presence of several well separated systems within a sample may cause discontinuities in the estimate of some structure-sensitive parameter along the Kittler sequence. On the other hand small scale fluctuations of the probability density characterizing the substructure within one system can cause the presence of different peaks close to one another and also some minor fluctuations in the parameter estimate.

7. An outline of the analysis

By exploiting the methods described in the previous sections we have designed a procedure that analyses the structure of a data sample which represents the three-dimensional positions of a set of point-like masses.

The analysis is divided in two parts. The first part considers only the geometrical structure ignoring the fact that the points we are considering form a dynamical system. In the second part we analyse the structure and substructure by considering their effects on the

³Here $f_{ka}(x, y)$ is the estimate of the probability density of the bimodal sample S .

estimate of a given parameter along a sequence of sample points ordered by non-increasing density within connected overdense regions.

Hence the final structure of the three-dimensional extension of DEDICA is the following:

1. analysis of the geometrical structure

- estimate the three-dimensional probability density function by the $f_{ka}(\vec{r})$ defined in § 2, and isolate the galaxy systems as peaks in $f_{ka}(\vec{r})$;
- estimate the cluster significance \mathcal{S}_μ of each system and the membership probability $P(i \in \mu)$ of each galaxy;
- apply the contact test; in the case that any systems are found to be in contact then apply a local whitening in order to correct $f_{ka}(\vec{r})$ for locally non-isotropic kernels.

2. analysis of structure and substructure effects

- by using the density estimate $f_{ka}(\vec{r})$ get the Kittler sequence \mathcal{K} and the plot of the KM:

$$\{(r_i, h_i)\} \rightarrow \{(k, f_{ka}(r_k))\} \quad (37)$$

- consider the following sequences: $M(k)$, $\sigma_V(k)$ and $R_V(k)$ obtained by estimating the virial mass, velocity dispersion and virial radius of the first k galaxies within the Kittler sequence \mathcal{K} ; also consider the plot of $\sigma_V(k)$ versus $R_V(k)$ which should indicate the presence of systems elongated along the line of sight (the fingers-of-God effect); use all these plots to infer information concerning the structure of the sample.

In the next section, we show the results obtained by applying the procedure outlined here when applied to two galaxy clusters taken from the literature.

8. A1656 (Coma)

This is a classical rich cluster. The data are taken from Kent & Gunn (1982) and were kindly provided to us in a computer readable form by Girardi et al. (1994). The list of the magnitude complete sample contains $N = 337$ galaxies brighter than 16.0. We have rejected

the galaxies with unknown magnitude. We want to examine the clustering structure in this quasi-three dimensional space, taking V as the radial polar coordinate.

In order to have homogeneous coordinates, for the present cluster and for the following one, we transform the (α, δ, V) set to the equivalent cartesian coordinates (x, y, z) , by:

$$\begin{cases} x = V \cos(\delta) \cos(\alpha) \\ y = V \cos(\delta) \sin(\alpha) \\ z = V \sin(\delta). \end{cases} \quad (38)$$

In Fig. 15 we plot the (x, y) positions of the galaxies in this sample. Contrary to the visual impression given by Fig. 15 and later by Fig. 24, we have decided not to blindly whiten the data, but to apply the whitening procedure only when the contact test is positive as is suggested by the discussion in § 4. By applying the three-dimensional version of DEDICA to this data sample, we have detected the presence of $\nu = 56$ clusters plus $n_0 = 84$ isolated galaxies. Among these clusters 22 have $0.90 \leq S_\mu < 0.99$ and are listed in table 4 while 13 have $S_\mu \geq 0.99$. The contact test shows the presence of only weak contact, moreover in no case have we obtained unimodal systems after the merging. Because of this reason we do not consider the whitening of the data. Hence it seems that the A1656 sample contains a rich collection of geometrically disjoint systems (see Fig. 16). This indication is supported also by the Kittler map (see Fig. 17) where the peaks indicating the significant clusters are separated by points at rather low density values. In fact from Figs. 16 and 17 it can be seen that A1656 consists of a very dense system surrounded by several satellite clusters at nearly 1/4 or 1/5 of the peak density (see also Fig. 18). The first two peaks in the Kittler map are due to the clusters $\mu = 31$ and $\mu = 32$ which are also in contact (see table 5). These results suggest that A1656 has a structure consisting of a bimodal core and an extended halo.

A bimodal structure in the centre of the Coma cluster has also been found in previous studies (see, for example, the results obtained by Fitchett & Webster (1987), Mellier et al. (1988)). Our result supports the conclusions of Fitchett & Webster (1987) and is more general since it is not constrained to detect only bimodal structures as does the Lee statistics. (see §1 and paper I). The large number of local peaks found by Mellier et al. 1988 is also in agreement with our results, although these authors have used mainly bi-dimensional data. On the other hand, several authors (see e.g. Dressler & Schectman 1988; West & Bothun 1990) have found no sign of significant substructure in the Coma cluster. This disagreement is probably due to the particular definition of the statistics which they have adopted in order to detect substructures.

Concerning the comparison between the presence of structure derived from optical data and the smooth appearance of the x-ray brightness distribution, it is possible to note (Fitchett 1990) that x-ray emission from the gas traces the gravitational potential in the standard hydrostatic model. Since the galaxy distribution is linked to the gravitational potential through the Poisson equation, it is not unreasonable that the x-ray gas distribution is smoother than the galaxy distribution.

Structure and substructure effects

In Figs. 19a,b we show the plot of the virial mass $\log M(k)$ and its dispersion $\Sigma[M(k)]$ estimated following the Kittler sequence. It is possible to distinguish at least three regions in $\log M(k)$. The first region goes from $k = 1$ to $k \sim 34$. We call this region the core of the cluster. It is mainly due to the presence of the two groupings: $\mu = 31$ that extends up to $k = 18$, and $\mu = 32$ that covers the main part of this region. The smooth dependence of M on k passing from one cluster to the other indicates that the presence of these two clusters is probably due to substructure. We have also applied the pairwise Newton test (see e.g. Beers, Geller & Huchra 1982) to these clusters. The result was that

$$\frac{V_p^2 R_p}{0.76G(M_{31} + M_{32})} \simeq 2.1$$

Hence this suggests that the two clusters are unbound. However this test assumes that the clusters are point-like masses and this is probably not reasonable for extended systems which are in contact such as $\mu = 31$ and 32. The mass of the core is estimated as $\log M_c = 12.94 \pm 0.02$ in solar units (here and in the following the error estimates are obtained by using the jack-knife method). This value is roughly consistent with the upper limit of the core mass estimated as $\log M_c \leq 12.7$ by Kent & Gunn (1982). However, we note that their estimate is model dependent and considers only the galaxies within 3° of the centre whereas we have considered all of the galaxies and our mass estimate is model-independent. Beyond $k \sim 34$ and up to $k \sim 300$ the slope of M versus k changes significantly. The plot of $\sigma_v(k)$ versus $R_V(k)$ (Fig. 20) shows the presence of several "fingers-of-God": regions where the value of the virial radius R_V stays roughly constant, while the velocity dispersion σ_v grows. The last finger terminates roughly at $\sigma_v \sim 950 \text{ Km/s}$ (i.e. at $k \sim 300$). This suggests to us that probably the outer limit of the cluster occurs at this value of k .

These results suggest that this region may be composed of satellite clusters distributed around the dense central core of A1656. Let us call this region the halo. The mass of the core and halo is estimated as $\log M_{c+h} = 14.904 \pm 0.003$ in solar units. The best-fit estimate

of the mass of the cluster given by Kent & Gunn (1982) is $\log M_{c+h} = 15.10$, again not very different from our estimate. Moreover, by using both optical and x-ray data, Hughes (1989) obtained a value of $M = (1.85 \pm 0.24) \times 10^{15} h_{50}^{-1} M_{\odot}$ corresponding to $\log M = 14.97$ in our units. This is again in rather good agreement with our estimate.

We must state clearly that the values of the virial mass which we quote are from blind application of the virial theorem. The mass estimates are more a rough number computed in order to compare our results with those in the previous literature. We plan to explore the possibility of exploiting the structure to infer a self-consistent dynamical model of these systems without being constrained by the assumptions of the virial theorem. A similar piece of work for spherically symmetric systems is that of Merritt & Shaha (1993).

Finally, for $k \geq 300$, the slope of $M(k)$ increases and this may be due to background or foreground galaxies which are not linked to the cluster.

The above discussion is confirmed by the plots of the velocity dispersion $\sigma_V(k)$ and of the virial radius $R_V(k)$ versus k (Figs. 21a and 22a) as well as by the plots of $\Sigma[\sigma_V(k)]$ and $\Sigma[R_V(k)]$ versus k (Figs. 21b and 22b) along the Kittler sequence. In fact from $\sigma_V(k)$ (Fig. 21a) it is possible to notice the presence of a region with low dispersion and relatively low value of the jack-knife uncertainty $\Sigma(\sigma_V)$. This region extends out to $k = 34$ where $\sigma_V(k)$ versus k shows a quick decrease in slope and a quick rise of $\Sigma(\sigma_V)$. Within this region the virial radius grows until $k \sim 20$, beyond this value R_V levels to $\sim 1h \text{ Mpc}$. This is the central ($k \leq 34$) high density, low dispersion region we can call the core.

For $k \geq 34$ the values of both σ_V and R_V grow quite smoothly with k indicating that as we move along the Kittler sequence towards galaxies falling in regions of lower and lower density, the system expands both in the radian direction and in the plane normal to the line of sight. It turns out that along the line of sight the structure of the sample is unimodal and characterized by a single peak at 7000 Km/s (see Fig. 23). As k grows along \mathcal{K} we move from the high density peak of $f(V)$ towards the low density wings of $f(V)$. This fact causes the value of σ_V to grow smoothly with k and $\Sigma(\sigma_V)$ to decrease. On the other hand, the structure on the plane tangential to the celestial sphere is multimodal and this causes the value of $\Sigma(R_V)$ to fluctuate quite widely. This occurs until roughly $k \sim 150 - 170$. Beyond this value of k the value of R_V stops growing and $\Sigma(\sigma_V)$ has a minimum. This can be interpreted by saying that for larger k (and hence lower density threshold) the system expands mainly along the line of sight and hence the projected size of the system estimated by R_V stays constant while its uncertainty $\Sigma(R_V)$ decreases. On the other hand both σ_V and $\Sigma(\sigma_V)$ grow smoothly due to the fact that in this part of the Kittler sequence the galaxies fall in the low $f(V)$ wings. Finally at roughly $k \sim 300$ R_V begins to grow with k , moreover both σ_V and $\Sigma(\sigma_V)$ grow rather steeply with k . This is a reasonable indication

that we are now out of the halo of the Coma Cluster and including field galaxies.

9. The Cancer cluster

As an example of a multimodal cluster, we have considered the Cancer cluster. The data are taken from Bothun et al. (1983) where positions and redshifts are listed for $N = 123$ galaxies whose positions are shown in Fig. 24. The three-dimensional geometrical analysis of DEDICA shows the presence of $\nu = 24$ clusters and $n_0 = 32$ isolated galaxies (see Fig. 25). Among these clusters there are 6 with $0.80 \leq \mathcal{S}_\mu < 0.90$, 6 with $0.90 \leq \mathcal{S}_\mu < 0.99$ and 5 with $\mathcal{S}_\mu \geq 0.99$ (see table 6). We must stress the fact that the galaxies classified by DEDICA as clusters $\mu = 10$ and $\mu = 16$ are not considered in the clustering analysis by Bothun et al. (1983) since they clearly appear to be foreground projections. However we decided to include these galaxies in the sample and let DEDICA show that they are actually foreground objects. The contact test shows the presence of weak asymmetric contact of strength $\mathcal{L} = 0.12$ between $\mu = 10$ and $\mu = 16$. Hence the clusters found by DEDICA are rather well disjoint. As for A1656 the merging and whitening of the overlapping systems do not give unimodal systems. Hence we do not consider whitened data. The multimodal structure of this sample is well shown by the Kittler map in Fig. 26 where the highest peaks are associated with the significant clusters and appear to be separated by low density regions (see also Fig. 27).

Comparing the results obtained by DEDICA and those of Bothun et al. (1983) it is possible to say that there is only qualitative agreement. In fact Bothun et al. (1983) found a large group which they call A with $n_A = 38$ members plus four more groups with $n_B = 6$, $n_C = 9$, $n_D = 7$ and $n_E = 10$ members. With the exception of $\mu = 10$, all the significant groups (i.e. those having $\mathcal{S}_\mu \geq 0.99$) found by DEDICA (namely $\mu = 11, 12, 13, 19$) are contained within the A group of Bothun et al. (1983). Hence the A group shows the presence of significant substructure according to our analysis. A similar conclusion holds for the remaining groups B , C , D and E . In fact they are superpositions of one or two marginally significant groups (i.e. having $0.90 \leq \mathcal{S}_\mu < 0.99$) and of some nearby fluctuations of the density field.

Structure and substructure effects

We have performed the Kittler mapping for several clusters assuming the highest density galaxy of each cluster as the starting point of the Kittler sequence.

The easiest cluster to begin with is the foreground cluster $\mu = 10$. The Kittler plot $M(k)$ shows a very sharp break in slope at $k = 10$, while there is a smooth change of $M(k)$ passing from $k = 6$ that marks the end of $\mu = 10$ to the range $k \in [6, 10]$ that is occupied by $\mu = 16$. This suggests that the existence of two different structures ($\mu = 10$ and $\mu = 16$) instead of only one is due to substructure. The pairwise Newton test between these clusters indicates that they are mildly unbound. However due to the contact between these structures the hypotheses underlying this test are probably not satisfied. A blind application of the virial theorem gives the mass of this unit ($C_{10} \cup C_{16}$) as $\log M_{10+16}/M_{\odot} = 12.10 \pm 0.07$.

The remaining four significant structures $\mu = 11, 12, 13$, and 19 are well disjoint and satisfy the pairwise Newton test. Moreover in the $M(k)$ plot (Fig. 28a) the curve seems smooth out to $k = 22$ while beyond this limit the slope of $M(k)$ rises. A blind application of the virial estimator would give a mass of $\log(M/M_{\odot}) = 13.51 \pm 0.02$.

The plot of $\sigma_V(k)$ versus $R_V(k)$ is shown in Fig. 29. It is possible to notice the lack of prominent vertical sequences of points (the finger-of-God effect) supporting the multimodal structure of this sample.

The group B is found by DEDICA to be composed of the weakly significant cluster $\mu = 14$ together with $S_{14} = 0.86$ and three isolated galaxies. According to the Kittler mapping, the $M(k)$ curve shows a break at $k = 6$ with $\log M(k = 6) = 12.95 \pm 0.09$. The six galaxies are the members of $\mu = 14$ plus three isolated galaxies, however these additional members are not the same galaxies that Bothun et al. (1983) attribute to this structure.

The group C appears to comprise galaxies attributed by DEDICA to $\mu = 17, 18$ and 20 . The most significant cluster among these is $\mu = 18$ that has $\log M(k = 5) = 11.7 \pm 0.3$.

The group D is made essentially by the clusters $\mu = 4$ and $\mu = 8$. These two clusters are indicated by our analysis as probably being subunits of a larger structure with $\log M(k = 8) = 12.8 \pm 0.1$.

Finally the group E corresponds in part to the clusters $\mu = 7$ and $\mu = 9$ which seem to form a bound structure with $\log M(k = 12) = 12.80 \pm 0.07$.

We note that the values of the mass that we obtain for the clusters mentioned are almost two orders of magnitude smaller than the estimates given by Bothun et al. (1983). This discrepancy is due mainly to the presence of interlopers in the Bothun et al. (1983) groups and slightly to a difference in the definition of virial radius (see the definition in e.g. Pisani et al. 1992).

Concerning the plots of σ_V , R_V and $\log(M)$ with their uncertainties $\Sigma(\sigma_V)$, $\Sigma(R_V)$

and $\Sigma(\log M)$ versus k we can say that the virial mass shows the same shape as in the case of A1656, but with a very different slope. In fact at $k = 120$ the mass of Cancer is two orders of magnitude larger than in the A1656 sample. Moreover, there is some indication of fluctuation in the slope at $k = 15$ and 22 . The main differences relative to the A1656 sample are linked to the velocity structure and to $\sigma_V(k)$ and $R_V(k)$. In Fig. 30 we show the velocity structure of Cancer. It is possible to notice the presence of 5 peaks. Two of these are highly significant ($S \geq 0.999$); the first is centered at 2009 Km/s and contains 11 members while the second is centered at 4887 Km/s and contains 91 members. Moreover in the first peak of $f(V)$ we find the clusters classified as $\mu = 10$ and $\mu = 16$ by the three-dimensional analysis, while in the peak centered at 4887 Km/s we find $\mu = 11, 12, 13$ and 19 . The velocity dispersion σ_V grows quite smoothly with k (Fig. 31a). The value of $\Sigma(\sigma_V)$ has a minimum at $k \sim 50$ (Fig. 31b). For $k \geq 90$ the Kittler sequence includes members of different peaks causing both σ_V and $\Sigma(\sigma_V)$ to increase. Moreover R_V is rather constant for $k \leq 20$, while it grows almost steadily for the remaining part of the sequence (Fig. 32a). A short plateau may be noticed centered at $k \sim 100$. Hence apart from the first 20 members of \mathcal{K} for which the system develops along the line of sight, the Kittler sequence shows that the structure develops in both directions parallel and normal to the line of sight. Moreover there is evidence of significant structure both in velocity and in plane normal to the line of sight as also suggested by the fluctuations in $\Sigma(R_V)$ (see Fig. 32b).

In conclusion DEDICA shows the presence of at least two independent structures. None of these are free of significant substructure.

We may say that our analysis is in qualitative agreement with the results obtained by Bothun et al (1983) since we detect the presence of several geometrically and probably also dynamically unrelated structures. However the details of the clustering pattern that we found is rather different from that found by Bothun et al. (1983).

10. Summary and conclusions

In this paper we have confronted the problem of extending to the general multivariate case the clustering algorithm called DEDICA which was introduced by Pisani (1994) for univariate problems. The extension is in principle straightforward as several numerical simulations have shown. Moreover we have proposed a method that allows us to estimate the locally optimal metric and which hence improves the performance of the density estimator by reducing the noise in the gradient of the density. The method proposed basically rests on the assumption that a highly elongated structure is broken into several subsystems due to the sphericity of the kernels. These subsystems lie quite close to one

another. We have introduced a non-parametric estimate of the contact between these subsystems. After the merging of the significant systems that are in mutual contact we can estimate the locally optimal metric and significantly reduce the noise. Several tests on Monte Carlo simulations have supported the effectiveness of this method for both two and three-dimensional data samples.

Parallel to this noise reduction method, we have used a slightly modified version of a procedure called Kittler mapping for building a sequence of the data in the sample allowing us to show in a two dimensional plot the structure of a multidimensional data sample. We have used the Kittler mapping both to support the geometrical analysis of DEDICA and to obtain information about the effects of the structure detected within the sample. In fact, we have shown by using some examples that along the Kittler sequence the estimate of a given parameter (such as, for example, the coordinate dispersion σ) as a function of the number of particles considered, makes a quick change in slope when significant and large-scale structures is present. On the contrary the chosen parameter changes quite smoothly if significant but small-scale structure is present within the sample. We can say that a sample has substructure if only small-scale structure is present, while it has structure if large-scale structure is present. Further application of the Kittler mapping for dynamical purposes on larger sample is in progress.

In summary we have presented a general method of cluster analysis which is based on the estimate of the probability density of the data sample and which satisfies the following requirements:

- it does not require assumptions to be made concerning the number of members or any other feature of the systems it is designed to look for;
- it gives an estimate of the statistical significance of each system it detects: this is a useful number in order to distinguish likely systems from noise fluctuations;
- it gives an estimate of the membership probability for each point in the data sample to each detected system; this quantity can indicate the presence of interlopers within the detected systems;
- finally we have suggested a possible way to analyse the effects of structure and substructure on the estimate of the cluster's parameters;

In this framework we think that the disagreement concerning the definition, presence and relevance of structure and substructure within galaxy clusters (compare e.g. Fitchett & Webster 1987 with West & Bothun 1990) can be faced successfully.

In order to illustrate the performance of the method, we have applied the three-dimensional version of DEDICA to two different clusters: a rich unimodal cluster (Abell 1656, namely Coma) and a multimodal cluster (Cancer). Our results indicate Coma as a core-halo structure formed by a rather large number of geometrically distinct structures. For Coma, a rough quantitative agreement is obtained with previous studies based on optical (e.g. Kent & Gunn 1982) and both optical and x-ray (Hughes 1989) data. On the other hand, the Cancer cluster results composed of at least two distinct structures both with substructure. In the case of Cancer, only qualitative agreement is obtained with the previous literature (Bothun et al. 1983). We emphasize that our estimate of the clustering structure is obtained without making any assumption about the structures or any model concerning their properties.

Currently ongoing and future observational projects will provide new and rich data samples of galaxy clusters particularly suitable for the analysis presented here. Moreover we plan to use the results of the geometrical structures to infer a self-consistent dynamical model of these systems in a very general way without being necessarily constrained by the assumptions of the virial theorem.

We plan to extend the application of DEDICA to large scale galaxy samples in order to analyse structures on larger scales than galaxy clusters. Moreover, as an application of the non-parametric and hence model-independent estimate of the density we plan to estimate the topological properties of constant density surfaces estimated from rich galaxy samples.

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Fig. 15 The A1656 data sample: projection of the galaxy positions onto the (x, y) plane.

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Fig. 32 Plot of values estimated along along the Kittler sequence of the Cancer data sample for a) the virial radius $R_V(k)$, and b) the jack-knife estimate of the dispersion $\Sigma[R_V(k)]$.

Table 1: Values of Δ (eq. [29]) that result from the $N_s = 1000$ Monte Carlo simulations test with $N_p = 500$ of the performance of the density estimators for three values of the axis ratio a/b .

	$a/b = 1$	$a/b = 0.5$	$a/b = 0.1$
$\min\{\Delta\}$	1.42×10^{-5}	4.34×10^{-5}	8.26×10^{-4}
$\max\{\Delta\}$	5.87×10^{-4}	9.37×10^{-4}	5.64×10^{-3}
$\text{median}\{\Delta\}$	5.74×10^{-5}	1.00×10^{-4}	1.43×10^{-3}
$\Delta_{0.25}$	2.91×10^{-5}	7.88×10^{-5}	1.26×10^{-3}
$\Delta_{0.75}$	4.93×10^{-5}	1.43×10^{-4}	1.65×10^{-3}
$\text{mean}\{\Delta\}$	4.81×10^{-5}	1.30×10^{-4}	1.50×10^{-3}
$\text{st.dev.}\{\Delta\}$	6.28×10^{-5}	1.52×10^{-4}	1.58×10^{-3}

Table 2: The cluster parameters and significance for the MC simulated data shown in Fig. 3 (see § 4).

μ	n_μ	\bar{x}	\bar{y}	σ_x	σ_y	\mathcal{S}_μ
0	0	-	-	-	-	-
1	14	0.78	0.77	0.11	0.09	> 0.999
2	10	-0.68	-0.56	0.08	0.04	> 0.999
3	2	-3.06	1.40	0.06	0.15	0.466
4	2	1.31	-0.98	0.07	0.14	0.492
5	3	1.61	1.54	0.02	0.01	0.981
6	3	-0.44	1.52	0.23	0.01	0.856
7	6	-1.67	1.13	0.19	0.27	0.716
8	9	1.19	1.14	0.12	0.12	> 0.999
9	26	-0.05	-0.04	0.13	0.16	1.000
10	4	1.06	-2.03	0.15	0.33	0.651
11	3	0.23	-2.81	0.17	0.17	0.755
12	14	-0.99	-0.89	0.21	0.12	> 0.999
13	4	-0.59	-2.42	0.11	0.26	0.811
14	14	0.44	0.40	0.11	0.12	> 0.999
15	6	-1.02	0.30	0.22	0.29	0.857
16	6	-2.08	0.40	0.25	0.24	0.747
17	19	-0.42	-0.38	0.08	0.14	1.000
18	3	-2.34	-0.86	0.12	0.14	0.605
19	12	0.22	-0.69	0.35	0.27	0.991
20	3	1.49	0.36	0.10	0.20	0.745
21	3	0.23	1.15	0.06	0.28	0.682
22	5	-0.10	-1.61	0.31	0.07	0.819
23	9	-2.69	-2.04	0.31	0.50	0.734
24	3	-2.89	0.63	0.14	0.19	0.792
25	2	-2.88	-0.34	0.14	0.15	0.782
26	13	-1.71	-2.08	0.21	0.50	0.956

Table 3: The contact among clusters of the Monte Carlo simulation shown in Fig. 3 (see §4).

μ, λ	n	$\mathcal{L}(\mu, \lambda)$
$1 \leftrightarrow 8$	7	0.81
$1 \leftrightarrow 14$	10	1.52
$2 \leftrightarrow 17$	15	2.45
$2 \leftrightarrow 12$	8	0.65
$9 \leftrightarrow 17$	16	1.52
$9 \leftrightarrow 14$	10	1.01
$9 \rightarrow 19$	1	0.09
$17 \rightarrow 19$	1	0.04

Table 4: The mean parameters and significance of the clusters in the *A1656* region. Only the clusters with $\mathcal{S}_\mu \geq 0.95$ are reported

μ	n_μ	\bar{V}	σ_V	$\log(M)$	\mathcal{S}_μ
0	84	-	-	-	-
4	3	6637.	56.15	11.31	0.965
11	5	1186.	39.30	11.54	0.999
15	3	6872.	35.10	11.84	0.964
19	4	7543.	75.12	12.06	0.966
23	4	6175.	36.34	11.91	0.966
25	5	7228.	21.57	11.26	0.998
27	3	5516.	10.01	10.68	0.969
28	6	8009.	25.11	11.47	0.998
29	3	7703.	16.64	11.20	0.958
31	18	6837.	52.78	11.75	1.00
32	8	6671.	39.65	11.73	> 0.999
34	5	5369.	52.82	11.93	0.982
36	3	7194.	14.47	10.67	0.994
37	4	7604.	28.71	11.49	0.990
39	18	7556.	51.55	12.16	> 0.999
40	5	8179.	47.91	12.15	0.962
42	6	6026.	47.38	11.90	0.998
43	7	5663.	52.39	12.13	0.999
44	17	7068.	70.29	12.49	> 0.999
46	7	6375.	66.07	12.12	0.995
47	13	7834.	68.77	12.43	> 0.999
48	3	6642.	12.12	11.00	0.955
49	9	5888.	56.43	12.25	0.998

Table 5: The contact among clusters in the A1656 region.

μ, λ	n	$\mathcal{L}(\mu, \lambda)$
$29 \leftrightarrow 37$	2	0.28
$25 \leftrightarrow 36$	2	0.20
$31 \leftrightarrow 32$	3	0.20
$18 \rightarrow 39$	1	0.15
$29 \rightarrow 47$	1	0.01

Table 6: The mean parameters and significance of the clusters in the Cancer region

μ	n_μ	\bar{V}	σ_V	$\log(M)$	\mathcal{S}_μ
0	32	-	-	-	-
1	3	4147.	57.42	11.60	0.947
2	2	7501.	41.01	12.24	0.643
3	2	4629.	38.89	12.27	0.558
4	5	3512.	97.02	12.56	0.948
5	3	4281.	35.23	12.03	0.813
6	2	5706.	36.77	11.85	0.834
7	6	4153.	81.72	12.38	0.979
8	3	3763.	43.88	11.80	0.791
9	3	3911.	57.50	12.31	0.736
10	6	2130.	39.50	11.53	0.999
11	9	5042.	107.37	12.43	> 0.999
12	5	4837.	18.27	10.91	> 0.999
13	6	4692.	40.46	11.57	0.998
14	3	6511.	37.31	12.01	0.861
15	2	7552.	64.35	12.01	0.627
16	4	2020.	46.74	11.60	0.978
17	2	5588.	89.09	12.60	0.357
18	5	5340.	44.84	11.72	0.987
19	10	4461.	65.50	12.44	0.998
20	2	6200.	20.51	10.49	0.939
21	2	4590.	91.92	10.87	0.854
22	2	4712.	28.28	11.72	0.841
23	2	1298.	23.33	11.83	0.648
24	2	5102.	46.67	11.63	0.811